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ARPA-E MEITNER
eVinci Resource Team

Task 1: Evaluation of M&S tools for micro-reactor concepts

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1 Executive Summary

1.1 WEC Resource Team Task 1

The M&S requirements for reactor design evaluation are making use of multi-physics codes to demonstrate self-regulation in heat pipe reactors. The defining physics require the coupling of three discrete simulation spaces: a master thermo-mechanical FEM code (e.g. `ANSYS`, `MOOSE`, `ABAQUS`), a temperature and spatially dependent neutronics code (e.g. `MCNP`, `Serpent`, `RATTLESNAKE`, `PROTEUS`), and a heat pipe boundary condition definition (e.g. `SOCKEYE`). Different toolsets can be compiled between the separate regimes to leverage the physics provided by each code (e.g. `ANSYS`+`MCNP`+`SOCKEYE`, `MOOSE` based animals). Since any given toolset can be justified in isolation, a set of metrics (e.g. robustness, accuracy, speed, availability) required for the problem at hand needs to be developed in order to assess the best code pathway. The Resource Team will establish evaluation criteria and determine the two or three best options based on the Design Team milestone schedule, desired simulation outcomes, and the cost associated with enhancing a prospective code for required use. This task will be executed over a series of teleconferences between the Resource Team members to assess the different modeling options.

Definition of Done: Establishment of evaluation criteria and determination of two or three M&S toolsets that could be used for reactor design in analysis in subsequent tasks

1.2 Summary

The Westinghouse Electric Company (WEC) and Los Alamos National Laboratory (LANL) have been awarded a DOE ARPA-E MEITNER award for development of its eVinci micro-reactor design. Fundamentally, the attractiveness of heat pipe micro-reactors comes from the idea that the core is inherently self-regulating, simplifying the reactor design and requiring significantly fewer safety related components. While the WEC Design Team is focused on the experimental and fabrication tasks to ensuring self-regulation, the MEITNER Resource Team is focused on utilizing available codes to computationally show the core is indeed self-regulating. This requires the combination of fundamentally different codes to simulate the feedback mechanism between heat generation, temperature, and density.

Simulating the defining physics of self-regulation in a heat pipe cooled micro-reactor requires the coupling of three discrete simulation spaces: a master thermo-mechanical FEM code (e.g. `ANSYS`, `MOOSE`, `ABAQUS`), a temperature and spatially dependent neutronics calculation (e.g. `MCNP`, `Serpent`, `RATTLESNAKE`, `PROTEUS`, or combination of several core physics codes), and a heat pipe boundary condition definition (e.g. `SOCKEYE`, `HTPIPE`). Different toolsets can be combined between the separate regimes to leverage the physics provided by each code (e.g. `ABAQUS` + `MCNP`

+ SOCKEYE, MOOSE based animals).

Due to the variety of different codes that could help address the problems at hand, the first task for the Resource Team has been to lay out the problem at hand and potential tool-sets that could be used to simulate the eVinci core. This document is the culmination of Task 1 and addresses:

- Overview of micro-reactor technology;
- Identification of problems to assess and metrics of success;
- Assessment of available codes and potential toolsets;
- Down-selection to two or three toolsets most likely to succeed;
- Definition of an initial assessment problem.

Each of the above bullets are explored in detail within this document, except for the last bullet which will be provided separately.

In general, heat pipe cooled micro-reactors all have the same key aspect that makes them so attractive, namely the ability to self-regulate due to strong thermal feedback effects. The eVinci reactor, like most heat pipe reactors, is comprised of a solid core block (SCB) that contains fuel rods, moderator rods, and heat pipes, in a triangular pitch. Thermal feedback is derived primarily from three separate physical phenomenon: 1) cross-section increases due to doppler broadening and shifts of the spectrum into regions with high resonances, 2) density changes due to thermal expansion, and 3) fuel pitch increases due to thermal expansion.

The primary goal of the Resource Team is to provide a set of codes and calculations to support the Design Team. As such, the tools utilized must appropriately solve the problems at hand, must be readily available for use, and provide continuing benefit to the Design Team during and beyond the MEITNER award period. While the Resource Team is primarily motivated by the question of self-regulation, the problems and goals of the larger project must be included in the initial code down-selection to be of maximum use to the Design Team.

During the exploration of codes in Task 1, it became clear that only the INL MOOSE-based tool-suite showed promise in producing results within the limited timeframe of the project. As a result, Task 2 will focus on the application of the INL codes to the assessment problem in order to force any complications and issues with the M&S to the surface early within the project such that appropriate resources could be redirected.

The Abaqus+MCNP toolkit will be used for independent comparison due to the familiarity of use with micro-reactors at LANL. It is not expected that the Abaqus+MCNP toolkit will be able to handle the complex analysis required to prove self-regulation of the eVinci core. In addition, although it is unlikely the Proteus+MOOSE tool-set will be able to provide coupled simulations with the limited project time, ongoing work with the toolkit will continue independently from MEITNER, may provide another independent assessment tool.

For Task 2, an assessment problem consisting of a unit assembly for a LANL design of a moderated micro-reactor will be used to exercise the MOOSE-based tool-set. Once success is shown with the smaller unit assembly, a full core of the LANL design can be used in place of better or protected information about the actual eVinci core.

2 Introduction

Westinghouse Electric Company (WEC) has been awarded an ARPA-E MEITNER award for development of its eVinci micro-reactor design. The reactor is comprised of a solid core block (SCB) that contains fuel rods, moderator rods, and heat pipes. A key aspect of the reactor design is the self-regulating nature due to the feedback between the heat generation in the fuel, the temperature of the moderator and fuel, and the density of core components.

The modeling and simulation (M&S) requirements for the eVinci reactor design evaluation is to make use of multi-physics codes to demonstrate self-regulation in heat pipe reactors. The defining physics requires the coupling of three discrete simulation spaces: a master thermo-mechanical FEM code (e.g. `ANSYS`, `MOOSE`, `ABAQUS`), a temperature and spatially dependent neutronics calculation (e.g. `MCNP`, `Serpent`, `RATTLESNAKE/MAMMOTH`, `PROTEUS`, `PARCS`), and a heat pipe boundary condition definition (e.g. `SOCKEYE`, `HTPIPE`). Different toolsets can be combined between the separate regimes to leverage the physics provided by each code (e.g. `ABAQUS` + `MCNP` + `SOCKEYE`, `MOOSE` based animals). Since any given toolset can be justified in isolation, a set of metrics (e.g. robustness, accuracy, speed, availability) required for the problem at hand needs to be developed in order to assess the best code pathway. The Resource Team will establish evaluation criteria and determine the two or three best options based on the Design Team milestone schedule, desired simulation outcomes, and the cost associated with enhancing a prospective code for required use.

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3 Micro-reactors

The eVinci micro-reactor concept is based on a long history of heat pipe micro-reactor development at Los Alamos National Laboratory [1, 2], culminating in a successful test of a kilowatt scale space reactor [3], and design of a megawatt scale terrestrial design [4]. WEC has teamed with LANL to develop a commercially viable reactor design that meets several key aspects [5]:

- Transportable energy generator;
- Fully factory built, fueled and assembled;
- Combined heat and power - 200 kWe to 25 MWe;
- Up to 600 °C process heat;
- 5- to 10-year life with walkaway inherent safety;
- Target less than 30 days onsite installation;
- Autonomous load management capability;
- Unparalleled proliferation resistance;
- High reliability and minimal moving parts;
- Green field decommissioning and remediation.

The eVinci reactor design overview is displayed in Fig. 3.1. The core monolith is a solid block of stainless steel or a similar advanced material with holes in a hexagonal pitch containing fuel, moderators, and axial reflectors. The monolith is connected by the primary and decay heat exchangers via heat pipes, thus defining the solid core block (SCB). In isolation, the SCB is subcritical, and requires radial and/or axial reflectors to achieve criticality. Beyond the inherent self-regulation, control drums embedded into the reflector can be used to control large reactivity adjustments. Lastly, a central safety rod can be used to shut down the reactor using passive control techniques.

Due the the proprietary nature of the eVinci design coupled with a shifting set of requirements, testing the Resource Team tools with a core design similar to an eventual eVinci reactor, but developed outside of the confines of information protection and changing economic landscapes, may simplify the analysis in the initial stages of development. An example of a core that could be used as a surrogate for the reactor core is the so-called “empire” design created by LANL [6], displayed in Fig. 3.2.

Given a combination of eVinci constraints and the empire core design, the following is a brief discussion about the major systems involved in micro-reactor core performance. Where available, the eVinci design parameters will be utilized.

3.1 Monolith

The monolith is a stainless steel block with cylindrical holes typically in a triangular pitch that contain the fuel, moderator, and heat pipes. As a result, the geometric integrity of the stainless

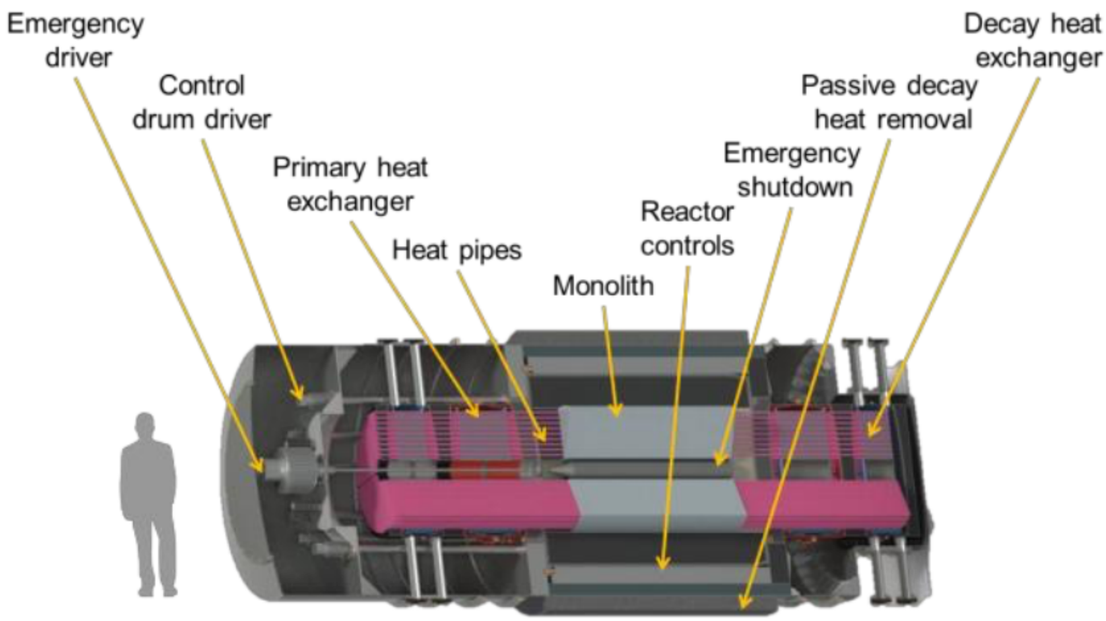


Figure 3.1: eVinci core overview [5]

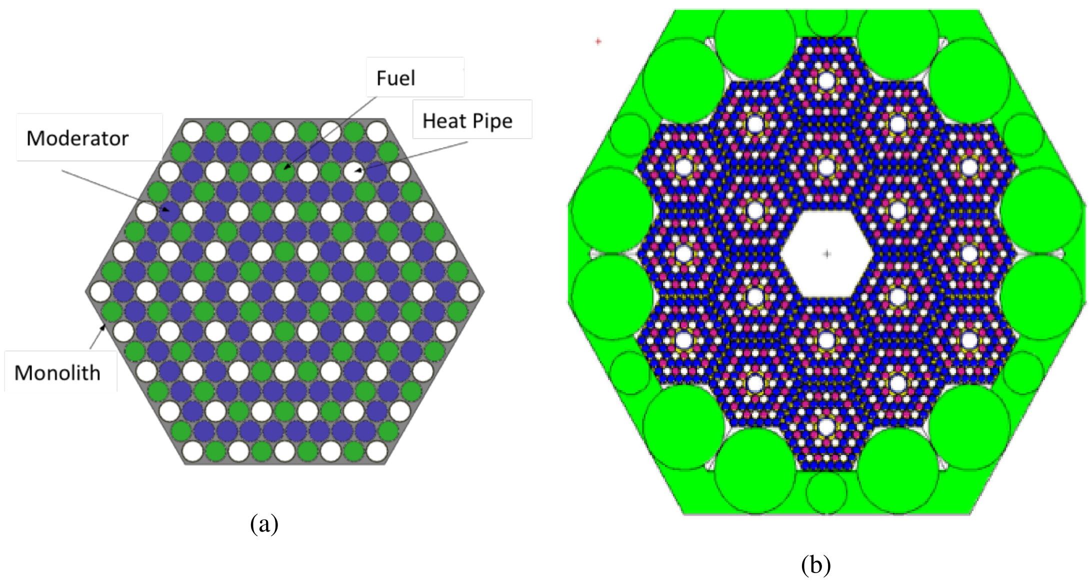


Figure 3.2: a) LANL empire unit assembly and b) core design [6]

steel monolith is essential for ensuring the safe operation of the reactor. Large deformations in the monolith can lead to operational and safety basis accidents such as;

- Fission product release - monolith deformation may lead to a pathway for release of gaseous radio-nuclides, either through mechanical failure of the fuel pin or separations in the monolith itself;
- Heat pipe failure - monolith deformation may lead to heat pipe failures, restricting the ability of the reactor to cool. While a small handful of heat pipe failures may prove to be accommodated, failure of several heat pipes in a close configuration can lead to large-scale failure of the reactor;
- Criticality issues - monolith deformation may place the core configuration in either a sub-critical or super-critical state, limiting operability of the core.

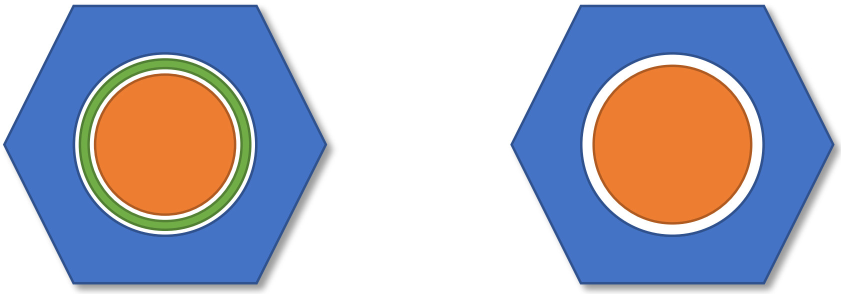
One of the major constraints related to the nuclear core design is the pitch or distance between adjacent fuel, moderator, and heat pipe rods. In the empire core design, the desired pitch results in a monolith minimum “webbing” widtch, or minimum thickness between adjacent fuel/moderator/heat pipe holes, of 1.5 mm. Given the temperature gradients across the webbing, stress relaxation via long-term creep may occur.

Although the broad design characteristics of the monolith are determined, the actual fabrication path for the monolith is still an open question. The Design Team will investigate two advanced manufacturing techniques, 1) vacuum diffusion bonding (VDM) and 2) laser additive manufacturing (LAM). Both fabrication techniques must adequately result in a monolith that retains the characteristics of its wrought counterpart, while maximizing advantages provided by the advanced techniques such as integral heat pipe structures built-in to the monolith. For the purposes of the simulations performed by the Resource Team, the monolith will be assumed to perform similar to a traditional single wrought piece. The fundamental basic design of alternating cylindrical holes filled with fuel, moderator, or heat pipes which form the reactor core will be retained independent of the fabrication technique.

3.2 Fuel

The nominal fuel system design is uranium nitride fuel (UN) in stainless steel cladding (Fig. 3.3a). The rods (fuel and cladding) will be fabricated independently and slid into the monolith. Due to the uncertainty of a stable UN fuel fabrication path, other fuels that are being investigated are uranium-zirconium metallic fuel alloys, uranium dioxide, uranium molybdenum, and uranium silicide fuel. In addition, the option of utilizing the monolith as a cladding itself is being explored, removing the extra layer of steel between the fuel and the monolith, as in Fig. 3.3b. In these integral type designs, a thin layer of zirconium metal may be included to prevent interaction between the fuel and the stainless steel monolith, however the liner will not be expected to retain radionuclides in the event of an accident.

Independent of the final fuel system design (individual or integral cladding), the contact between the fuel system and the monolith will need to be addressed. In general, mechanical contact tends to be a difficult problem for finite element simulations. Due to the possible swelling of the



(a) (b)

Figure 3.3: Pin sub-cell types with a) individual cladding and, b) integral cladding.

fuel in measurable amounts, frictional contact may be required for contact surfaces shared with the fuel. Otherwise, frictionless or glued contact may be able to adequately capture the strain interaction between thermally expanding parts.

In general, the power level of the core is low enough that total burnup will likely not exceed 1 a/o. As a result, micro-reactor fuel pins may be able to avoid the major micro-structural changes that high burnup fuel systems suffer from such as constituent redistribution, extensive swelling, and high fission gas release. Instead, the long service time of up to 10 years, and high temperatures between 500-600 °C can lead to fuel cladding chemical interaction (FCCI). This will especially be prevalent in metallic fuels such as U-Mo or U-Zr, motivating the use of liners to separate the monolith from the fuel.

3.3 Heat Pipes

Of the micro-reactor designs that are being pursued, those that use heat pipes for heat transfer are the most mature, primarily due to the success achieved with the space reactor tests [3, 4]. Heat pipes take advantage of boiling and condensation of a working fluid to transfer energy through the use of gaseous diffusion and capillary force. A heat pipe typically consists of a sealed metallic tube filled with a working fluid such as water, ammonium, or sodium. At the hot end of the heat pipe, thermal conduction through the tube boils the working fluid, which travels through the center of the tube. At the cold end of the heat pipe, the working fluid condenses, releasing latent heat. A mesh or ribbing structure along the inside diameter of the tube provides a wicking pathway that drives the condensed working fluid back to the hot side of the heat pipe. The extremely effective use of latent heat of the working fluid results in a highly conductive pathway for heat removal, providing over two orders of magnitude larger effective thermal conductivity than copper.

The heat pipes in a micro-reactor core consist of stainless steel encasements filled with a sodium working fluid. The MEITNER design team is actively pursuing cost effective fabrication of the heat pipes based on the extensive experience provided by the LANL team. Similar to the considerations of the fuel system, two heat pipe configurations are being explored for independent drop-in heat pipes, and integral heat pipes. Both types of heat pipes will utilize a double condenser configuration due to core configuration (Fig. 3.1).

In general, heat pipes provide a high level of confidence in robustness and repeatability due to the lack of moving parts and sealed design. The primary concern in heat pipe systems should be on any mechanism that results in a cascading common mode failure of a significant fraction of all heat pipes, which can lead to loss of reactor cooling. Cascade failure is the result of insufficient margin on the load carrying capability of a heat pipe such that when a neighboring heat pipe fails, the surrounding heat pipes are unable to carry the additional thermal load, and fail themselves. If a cascading heat pipe failure is unable to be terminated quickly, enough permanent damage to the heat pipes or reactor can occur, resulting in an inoperable core or failure of the monolith. Cascade heat pipe failure is most likely induced by failure of one or two heat pipes by other means enumerated below, or by the overloading of a heat pipe from a localized power anomaly.

Heat pipe failure mechanisms come in two classes, a) those that result in permanent failure of the heat pipe and b) those that limit the maximum performance of a heat pipe. In general, the items that cause permanent degradation or failure stem from external events such as:

- Collision or impact;
- Manufacturing defects (e.g. non-metallic impurities in working fluid);
- Radiolytic gas production (e.g. argon-38 production from potassium-39);
- Corrosion;
- Diffusion of non-metallic impurities leading to de-wetting;
- Closure failure (e.g. weld failure on the cap);
- Severe overheat (Several hundred degrees Celsius will lead to chemistry changes that can induce permanent failure).

Barring extreme cases, the operating envelope can be enclosed by five different regimes that result from combinations of temperature and power. Typically, these failures are recoverable via power or temperature adjustments back to an adequate operating envelope. A sample plot of these limits for a composite wick is show in the figure Fig. 3.4 and consist of:

- Viscous limit;
- Sonic limit;
- Capillary limit;
- Entrainment limit;
- Boiling limit.

Of these, the viscous and sonic limits are self-recovering if the system can afford the natural rise in temperature. The others will require intervention to recover.

The viscous limit is a low vapor-pressure condition that may exist during frozen start-up or reduced power operation. The viscous limit is benign and seldom leads to problems. At low temperature, the fluid driving force is the absolute vapor pressure in the heated zone, which is typically insufficient to overcome the friction pressure drop of fluid moving along the pipe length. Vapor cannot travel the whole length of the condenser, and an abbreviated active (isothermal)

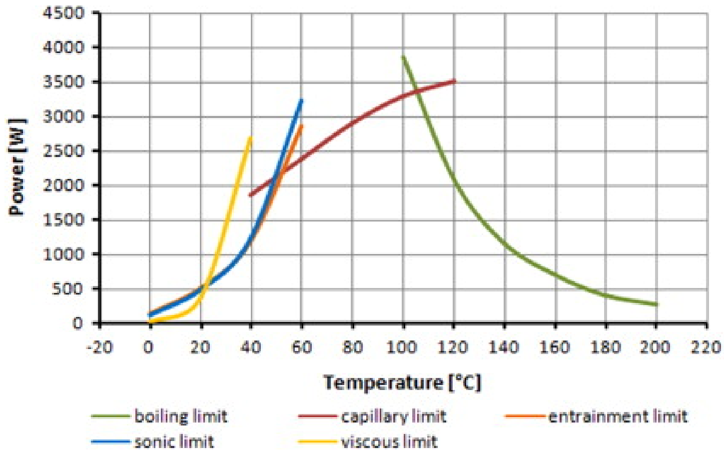


Figure 3.4: Sample performance limits for a composite wick heat pipe

region results. During operation at the viscous limit, heat transfer by vapor movement is of similar magnitude to axial heat conduction in the heat pipe wall. The vapor pressure increases as the heat pipe warms and becomes sufficient to circulate fluid. The viscous limit ends once the heat pipe becomes isothermal along its entire length.

The sonic limit occurs during start-up at a higher temperature than the viscous limit. Vapor cannot exceed the sonic velocity at the evaporator exit. Further heat input requires the evaporator end temperature to rise relative to the condenser end. Once the sonic limit is reached, the heat pipe temperature increases in response to further power increases. This benign limit does not normally lead to problems, and typically not a bad place to operate a heat pipe.

The capillary limit is the power level that produces mass flow rates sufficient for liquid and vapor pressure drops to exceed the maximum capillary head potential of the wick. In this limit, vapor flow leaving the evaporator exceeds liquid return, and the evaporator temperature rises from liquid depletion. Once the evaporator dries, power applied to the heat pipe must be reduced and its temperature lowered to allow condensate to rewet the wick. It is best practice to stay away from a capillary limit during normal operation as repeated journeys into this condition may lead to surface chemistry problems or even wick damage. Keeping the heat pipe twenty percent below an established capillary limit should avoid difficulties. In practice, annular wicks are seldom perfectly straight and can assume both concentric annular and crescent annular positions along the length of the heat pipe. Corresponding friction factors for fully developed laminar flow through eccentric annular ducts can be found in Rohsenow [7]. A concentric annular wick inside an alkali metal heat pipe can have a laminar flow friction factor ~ 2.5 times higher than a crescent annular wick. The liquid pressure drop through a concentric annulus is larger than the pressure drop through a crescent annulus, so simulation codes utilizing the concentric annulus approximation can frequently under-predict (conservative) the capillary limit by around 10%, for typical conditions.

Counter-flowing vapor may sweep liquid out of the wick and deprive the evaporator of returning liquid. This condition is called an entrainment limit. This limit is most common when high-velocity vapor flows over open grooves. Entrainment is seldom a serious problem in compound alkali metal heat pipe wick structures that shield the condensate from counter-flowing vapor. Very little study has been made of entrainment limits for alkali metal heat pipes.

Evaporation in an alkali metal heat pipe usually does not involve true boiling but instead surface vaporization. Liquid moves axially and preferentially in a skin next to the vapor core. At high evaporator radial heat flux vapor, high temperature, or in rough or dirty un-wetted systems, bubbles may form at the superheated wall. The wick can impede radial movement of bubbles from the heated wall leading to local drying and rapid evaporator temperature rise. Superheats possible before boiling onset in alkali metal heat pipes are large: typically over a hundred degrees Celsius. Silverstein's treatment of boiling in alkali metal heat pipes rings true and is recommended reading [8].

3.4 Moderator

The moderator used in micro-reactors must be able to withstand high temperatures due to the solid core block configuration. The nominal empire design utilizes yttrium-hydride in rodlet form, however zirconium-hydride is being considered as a back up material. In both types of moderator forms, temperatures must be kept below diffusion limits in order to ensure the hydrogen does not diffuse out of the rod, leading to ineffective moderation.

Although yttrium-hydride is the most attractive moderator for use in high temperature applications due to a relatively slow hydrogen mobility, there remains uncertainty in the thermalizing behavior of the hydrogen. The yttrium-hydride temperature reactivity coefficient as a function of time should be investigated and qualified.

4 Problem Requirements

Fundamentally, the attractiveness of heat pipe micro-reactors comes from the idea that the core is inherently self-regulating, simplifying the reactor design and requiring significantly fewer safety related components. While the WEC Design Team is focused on the experimental and fabrication tasks to ensuring self-regulation, the MEITNER Resource Team is focused on utilizing available codes to computationally show the core is indeed self-regulating. This requires the combination of fundamentally different codes to simulate the feedback mechanism between heat generation, temperature, and density.

A simplified flowchart of the four different codes and their connections is provided in Fig. 4.1. The primary driver code will be a finite element code that can capture the thermo-mechanical response of the core given the heat source generated in the fuel. The density and temperature information will then be utilized in a neutronics code in order to determine the fission source term. A code that captures the behavior of heat pipes provides the ultimate heat removal rate from the monolith. Lastly, a systems analysis code that captures system wide events such as start up, reflector drum manipulations, and secondary side heat removal will be an important consideration for the Design Team following the successful simulation of the self-regulating core. Due to the tightly coupled nature of the core, the three code domains must be solved either simultaneously, or more likely, via Picard iteration in order to fully capture the coupling of the different phenomenon. One directional coupling may be possible in conditions where temperature is not deviating significantly, but may miss the thermal feedback expected.

Given the natural separation of the physics, the phenomenon at hand can be separated into the respective codes. The details required by each code is combined into Fig. 4.2, while the coding requirements can be separated into two regimes, short and long term. These categories roughly correspond to what lies within the scope of the MEITNER Resource Team tasks (short term) and goals that are of interest to the Design team after, or concurrently with the MEITNER scope (long term).

The requirements for the modeling and simulation efforts in the near term are to show the self-regulating behavior of the core during 1) steady state operation and 2) during transient conditions. Since the self-regulation is directly tied to the temperature and density of the core, a coupled thermo-mechanical solve is required to capture self-regulation. This includes a driver finite element code to calculate the thermo-mechanical response due to heating from the fuel and cooling from the heat pipes, a neutronics code to calculate the source term, and a heat pipe code to calculate the energy removal rate. The core physics that must be captured can be separated into two regimes;

- Temperature distribution - This will drive the neutronics cross-sections and provide feedback to the fission source rate. Required components will be thermal conductivities of the materials, thermal contact models, heat pipe models to capture heat removal, and a heat pipe secondary-side boundary condition;

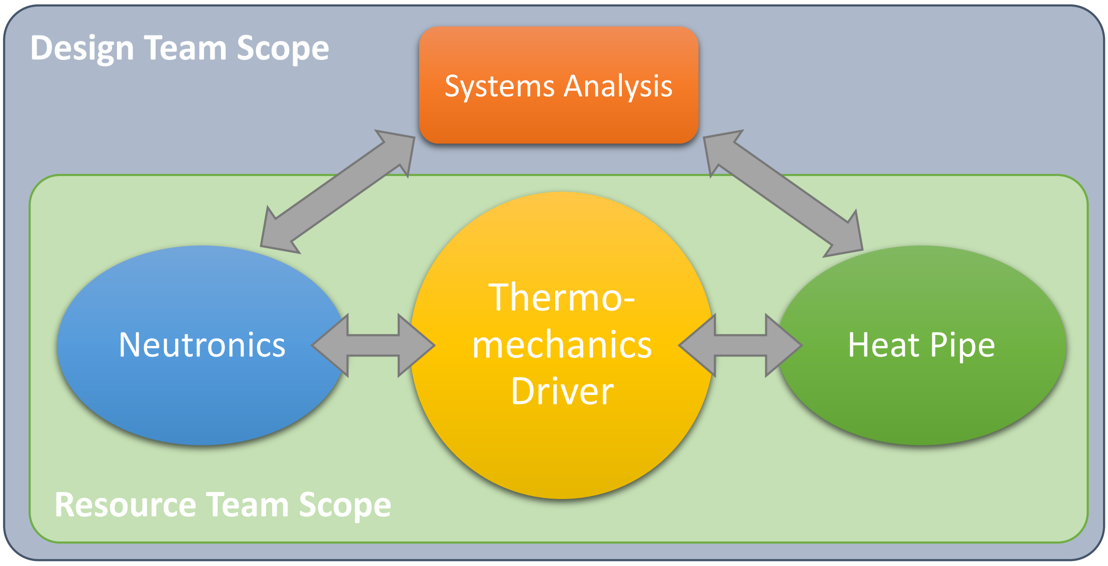


Figure 4.1: Overview coupling architecture for micro-reactors. The Design Team scope encompasses the Resource Team scope while adding systems analysis tools to the neutronics and heat pipe calculations.

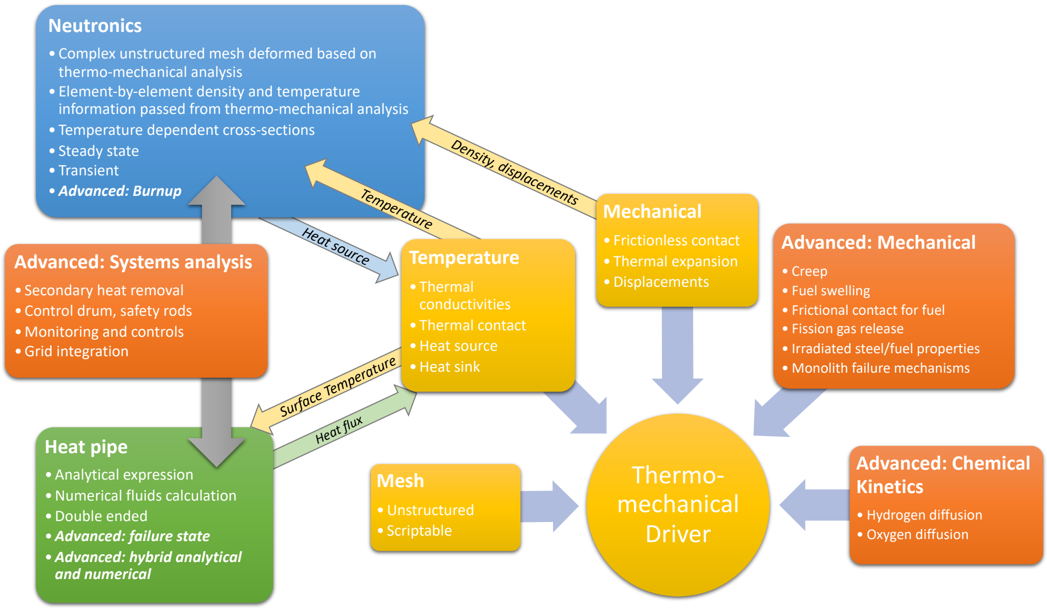


Figure 4.2: Expanded code architecture with the required problems to be solved by each code and through what mechanism each code will link. Items in orange are outside the scope of the Resource Team, but should be considered for future implementation into any tool-set that will be used by the Design Team.

- Mechanical deformation - Initially thermal expansion will be essential to capture the feedback to the fission source rate. Eventually, creep of the block will be required for long-term performance of the core. Contact models will be important to transfer the displacements between parts and capture any gap heat transfer coefficients.

In previous coupled simulations by LANL for small space reactors, the core design was simplified such that the swelling of any given component was isometric [9]. This allowed for the combinational geometry mesh traditionally utilized by Monte Carlo neutronics codes like `MCNP` to be utilized as any volumetric change in the mesh could be captured by simple dimensional changes. As the smaller heat pipe reactors are scaled up to larger terrestrial reactors, isotropic changes in the volume cannot be guaranteed due to separation of the core into different components (i.e. fuel, moderator, heat pipe) and regions. As a result, an unstructured mesh with element-by-element state variables for temperature and density is necessary to capture the complex geometric changes expected from the micro-reactor core.

Given that any thermo-mechanical finite element code generally focuses on the temperature distribution and mechanical deformation as a primary goal, the fundamental problem becomes linkage of the codes together in a coherent way. Figure 4.3 provides an example coupling regime between the codes, with the likely state variable communication paths in the red boxes. In principal, this requires the transferring of elemental temperatures, elemental densities, and nodal displacements from the thermo-mechanical driver code to the neutronics code, the elemental fission rate source from the neutronics code to the driver code, the heat pipe surface temperature from the driver code to the heat pipe code, and the heat flux from heat pipe code to the driver code.

The information passed between the thermo-mechanics and neutronics codes will likely be located on the same mesh. This will allow elemental state variables to be passed simply, but requires unstructured mesh capabilities from the neutronics code. The linkage between the thermo-mechanics code and heat pipe can likely be limited to state variables at the surface of the heat pipe.

The long term modeling and simulation goals should be discussed so that a useful tool can be provided to the Design team for use during and after the award period. Following the nuclear design modeling that will be attacked in the short term, the long term problems shift towards material performance and compatibility concerns;

- Monolith creep - The long term geometric stability of the core hinges on the creep resistance of the monolith. This is especially concerning at the monolith webbing, where the thickness is the thinnest;

- Secondary heat removal system coupling - The ability of the heat pipe to remove energy from the system is determined by the temperature at the hot side within the core, and the cool side condensers. The condenser efficiency is ultimately determined by the system it is coupled to such as super-critical CO_2 or an open-air Brayton cycle. Although initial testing by the Resource Team can utilize an analytical boundary condition on the heat pipe, eventual coupling via a systems analysis tool will help capture the true response of the system to external perturbations;

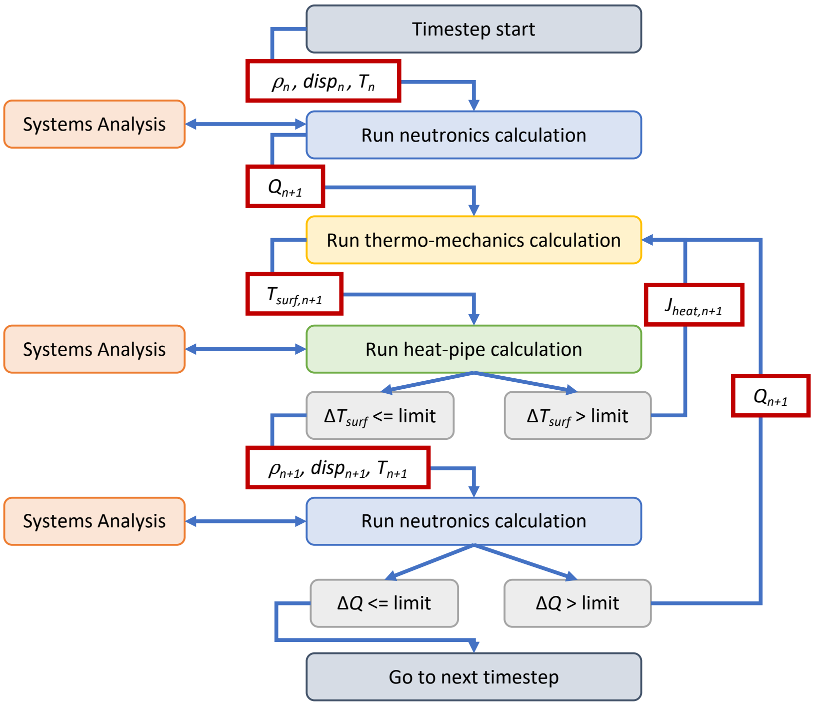


Figure 4.3: Psuedo-code of an example linkage system between the thermo-mechanical driver, neutronics, heat pipe, and systems analysis code. The likely communication paths between the codes are provided in the red boxes. The linkage path between the systems analysis code is not explicitly provided since they are likely numerous and outside of the scope of the Resource Team calculations.

- Fuel performance - Although the burnup of the core will be considerably less than traditional nuclear fuel, large swelling of metallic fuel has been observed in the past which can lead to large fuel-cladding mechanical interaction. Large axial growth can also lead to undesired reactivity changes that must be accounted for;
- Moderator performance - Yttrium hydride remains a largely untested moderator material. Hydrogen diffusion at high temperatures may become important during transient conditions, and must be taken into account for safety analysis;

External requirements must also be considered when defining the appropriate toolset for use. Due to the specific Resource Team mandate, limited resources will be spent for strict code development. This primarily is targeted to prevent large-scale code modifications, and is meant to focus the resource team on running simulations with development only limited to material definition implementations, simple model integrations, and code coupling via in-place mechanisms. As a result, the codes selected by the Resource Team must have a readily available community that is healthily funded by other means to rely on for any code development requirements that may evolve as the project continues. Codes with well established lines of communication and working relationships with the Resource and/or Design Teams are essential to prevent a dead-end M&S path. This requirement can be bolstered by the availability of source code to the Resource Team such that simple fixes can be implemented directly. If the source code is not available, the given toolset must explicitly demonstrate success for the problems at hand.

5 Codes

Given the considerations explored in Section 4, different codes can be explored to tackle the problems at hand. Included in each section is a brief overview of the applicable codes and a ranking tables that compares the different codes to the relevant success metrics (Tables 5.1 to 5.3).

5.1 Driver codes

5.1.1 MOOSE

The MOOSE framework is a finite element development platform built on the C++ finite element library libMesh [10] with the nonlinear solver package PETSc [11] in a developer friendly package. The primary aim of the code is to remove the computational engineering aspects of solving complex modeling problems by natively handling the vast majority of the numerical aspects of the code, including threading, MPI, I/O, and meshing, leaving the specific physics to the developer.

Since its inception, MOOSE has focused on providing a platform for coupling multi-physics calculations via tight (i.e. simultaneous solve) or loose (i.e. Picard iteration) coupling. This has been borne over the years as many different physics has been coupled via the common underlying MOOSE-framework between different physics applications [12–15].

5.1.2 ANSYS/ABAQUS

ANSYS and ABAQUS are commercial finite element analysis engineering packages which cover a wide range of mechanical engineering applications: stress & residual stain prediction, deformation, vibration characteristics, and stress induced creep. These tools help engineers to prepare the complex geometry and mesh direct from CAD files, to implement an adequate physics model into the computational domain of interest, and to help a series of optimization study based on the design objective function. A whole range of material models covering everything from hyper-elastics, shape memory alloys, concrete, and metallic structures can be accurately modeled. In addition, a handy user-defined material modeling capability is provided when the target simulating material is not available in the material database in the code.

In general, ANSYS and ABAQUS can handle physical models such as linear and non-linear dynamics, modal analysis, spectrum response and random vibration with pre-stress, and several contact models containing bonded, no separation, frictionless, frictional. In the transient domain both implicit and explicit solvers enable to model time dependent scenarios. Implementing an additional physics models such as creep model for fuel or fission gas induced swelling model

Table 5.1: Different driver codes compared to the relevant success metrics. ●= Readily available or otherwise best case scenario, ◐= adequate performance or model implementation, ○= not viable.

Metric	MOOSE	ANSYS	ABAQUS
Mechanical contact	◐	●	●
Thermal contact	●	●	●
Creep	●	●	●
Code Maturity	◐	●	●
Code Flexibility	●	○	○
Coupling Interface	●	○	○
Ease of use	●	●	●
Source code	●	●	●
Cost	●	○	○
Developer interaction	●	○	○
Massively Parallelizable	●	◐	◐
Run time	◐	◐	◐
Advanced capability implementation	●	◐	◐

are limited since users cannot gain access to the source code. However, applying user defined function on physics modification is available in some manner for both codes.

Simulations can be executed in a parallel computing platform if the model geometry is sophisticated and physics is complex. The entire solution phase runs in multi-cores architecture, including stiffness matrix generation, linear equation solving and results calculation in both shred and distributed memory processing. Unfortunately, the licensing structure for ANSYS and ABAQUS are such that each cpu requires an individual license based on a sliding scale such that large simulations can quickly consume an organizations license pool.

A weakly coupled calculation approach can be utilized between ANSYS or ABAQUS and a selected neutronics solver via I/O file transfer. For this type of coupling, input/output file parsing is achieved via python scripting between runs of each code. Even though tightly coupling feature is more desirable for a high-fidelity multi-physics calculation, ANSYS and ABAQUS do not allow these features at this point. However, a python script based weakly coupling method between ANSYS/ABAQUS and MCNP is already well demonstrated in various studies.

Although ANSYS and ABAQUS are well vetted and have been under development for decades, their source remains unavailable for modification. Still, there remains expert users both in industry and the national laboratories, however a risk remains with developing within these commercial codes as more advanced models may be unavailable in the coding structure.

5.2 Neutronics codes

5.2.1 MCNP

The Monte Carlo neutron transport code MCNP follows the statistical behavior of a large number of particles as they are transported through a system and can calculate accurate energy-dependent flux/power distribution and cross sections for numerous materials within a complex geometry such as nuclear reactor. The Monte Carlo method (such as that used in MCNP) simulates the actual process of particle transport stochastically by randomly sampling a large number of events [16]. Monte Carlo methods benefit from the fact that both continuous energy cross sections and detailed geometric modeling provide material- and system-dependent reaction rate behavior [17,18]. The Monte Carlo burnup code Monteburns, which links the Monte Carlo transport code MCNP to the isotope generation and depletion codes ORIGEN-S or CINDER90 [19–22] provides changes in isotopic compositions and other system parameters as a function of irradiation time using the energy-dependent cross sections and fluxes.

MCNP also calculates flux and thus power distribution in a system based on the number of neutrons traveling through a region of interest. It is important to have a well-validated code such as MCNP calculate three-dimensional power distributions and provide them to a thermo-mechanical and/or thermal hydraulic code to determine temperature distributions and other parameters. MCNP/Monteburns have demonstrated the ability to calculate power, flux, and compositions of over a thousand core materials as a function of irradiation [23]. MCNP also contains the ability to input an unstructured mesh geometry from ABAQUS (or in the near future BISON) for element-level evaluation. Iterations between MCNP and a thermo-mechanical code in terms of density, volume, temperature, and/or power of individual unstructured mesh elements will soon be possible.

MCNP uses ACE-formatted files, primarily from ENDF-based data and processed by the code NJOY as input cross sections. NJOY can process the files at a variety of temperatures, and Doppler-broadening treatment within MCNP can additionally handle temperature-dependence. MCNP has been well validated for many applications, including reactors and is robust and reliable on numerous computing platforms.

5.2.2 Serpent

Serpent is a Monte Carlo continuous-energy particle transport code developed at the VTT Technical Research Centre of Finland, Ltd since 2004 [24]. Similar to MCNP, Serpent has been utilized in nuclear reactor core , multi-physics coupling, and neutron source dose rate calculations. Serpent has been used in the past for coupled multi-physics simulations, including use as cross-section generation for RATTLESNAKE simulations.

5.2.3 OpenMC

OpenMC is a Monte Carlo neutronics code similar to MCNP, but developed with reactor modeling in mind and with an open-source license [25]. The code was originally developed by MIT, and is currently developed jointly by MIT and ANL. While the code has shown success with reactor modeling and coupling to finite element codes [14], unstructured mesh capabilities are not currently available. As the code base grows and unstructured mesh of the reactor geometry becomes possible, `OpenMC` shows promise in tackling the complex coupling problems at hand.

5.2.4 RATTLESNAKE

`RATTLESNAKE` is a `MOOSE`-based multi-group radiation transport application developed at Idaho National Laboratory (INL), for multi-physics modeling and simulations. `RATTLESNAKE` shares the `MOOSE` framework with various applications modeling other physics, which not only avoids functionality duplication among applications, but also enables more consistent data transfers for multi-physics simulations. `RATTLESNAKE` allows both strongly-coupled multi-physics calculations, where all physics reside in one equation system and are solved simultaneously, and tightly-coupled calculations where physics are solved sequentially with Picard iterations. `RATTLESNAKE` has been used for neutron, thermal radiation and phonon transport calculations. The design of `RATTLESNAKE` allows extension to other radiations straightforwardly.

A total of eight discretization schemes are available in `RATTLESNAKE` with continuous and discontinuous finite element methods (FEM) for spatial discretization and with diffusion, spherical harmonics expansion (PN) and discrete ordinates methods (SN) for angular discretization. All of them can participate the so-called multi-scheme calculations where schemes are applied on sub-domains and solved simultaneously for efficient computing resource management.

The unstructured mesh framework provided by `MOOSE` makes `RATTLESNAKE` highly flexible for analysis of various type of reactors. `RATTLESNAKE` can directly take the thermal expansion effect into account through the three-dimensional mesh displacement from solid mechanics. Pebble tracking transport algorithms are available in `RATTLESNAKE` for high-fidelity simulations of pebble-bed reactor analysis. `RATTLESNAKE` supports homogenization equivalence methods with super-homogenization, discontinuity factors and novel hybrid methods integrated in the multi-physics multi-scheme environment.

The design for flexible multi-physics, multi-radiation, multi-scheme tasks demands and ultimately makes `RATTLESNAKE` a highly extendable code system. A software quality assurance (SQA) procedure is enforced during `RATTLESNAKE` development.

5.2.5 MAMMOTH

`MAMMOTH` is a reactor physics `MOOSE`-based application that seeks to streamline the analysis of a variety of nuclear multi-physics engineering applications, including steady-state and unsteady core performance, fuel depletion, fuel performance, irradiation effects on core internals and RPV, criticality and decay heat calculations, reprocessing and non-destructive post-irradiation examination. This streamlining is accomplished via enhanced flexibility of the tools, uniform syntax in the `MOOSE` framework, dynamic linking of all relevant physics and a single-point of execution.

This enhanced flexibility of `MAMMOTH` as a reactor physics tool revolves around two key capabilities: 1) The Multi-Application (MultiApp) capabilities in `MOOSE`, which has created the opportunity for multi-physics simulations of nuclear reactors with varying levels of fidelity for each of the physics of interest and 2) recent technological advancements in the `RATTLESNAKE` multi-scheme methods, which allow various transport discretization to co-exist within the same solution space, thus allowing simulations with high-low fidelity in different regions of a domain of interest.

Improved depletion capabilities allow the needed flexibility to model low-resolution, core-wide depletion to the high-resolution required for the evolution of high-burnup structures (HBS). The number of depleting isotopes can vary from a few hundred to thousands, thus providing enough isotopic resolution for coupled or downstream calculations (i.e. fuel performance, decay heat). In addition, ANSI/ANS-5.1-2005 standard decay heat curves are supported.

`MAMMOTH` includes a variety of equivalence techniques including discontinuity factors, Super-homogenization as well as hybrid methods. The current generation of cross sections relies on external codes (e.g. `MCNP`, `Serpent`) but a `MAMMOTH`-native capability is underway based on well established, proven methods.

`MAMMOTH` currently boasts an unprecedented flexibility that allows the modeling of many reactor designs. `MAMMOTH` has been used in the modeling of PWRs (AP-1000, BEAVRS), TRIGA (NRAD), VHTRs (HTR-10, HTR-PM, HTTR, MHTGR-350), fast reactors (CEFR, VTR) and heat pipe reactors. Because of its inherent flexibility `MAMMOTH` is currently being applied in the transient analysis of both the TREAT.

5.2.6 PROTEUS

`PROTEUS` is a set of high-fidelity-capable advanced neutronics modeling and simulation tools including cross section generation codes, transport solvers (discrete ordinate (SN), method of characteristics (MOC), and NODAL), and mesh generation toolkit. The SN and MOC solvers are based on unstructured finite element meshes to be able to simulate complex geometries, while the NODAL solver can handle Cartesian and hexagonal geometries. All solvers can solve full transient problems. The code uses multi-group cross sections generated from `MC2-3` or Monte Carlo codes (`Serpent` or `OpenMC`), and can generate the self-shielded multi-group cross sections on-the-fly using the cross section API. Reactor geometry meshes for typical Cartesian or hexagonal assembly based cores can be easily generated using the mesh generation toolkit. The inputs to PROTEUS and the mesh generation toolkit are based on modern keyword-style text for ease of use. User and theory manuals are available.

The S_N solver operates on 2D or 3D unstructured finite element meshes (tetrahedral, hexahedral, prism, triangular, and quadrilateral element types available) which allows users to model any complex-geometry problems including thermal expansion or structural deformation. The MOC solver operates on 2D extruded meshes (quadrilateral and triangular element types available) to efficiently and accurately solve heterogeneous-geometry problems. Both solvers are massively parallel with reasonably good scalability. PROTEUS has been applied to experimental reactors (ATR, TREAT, RCF), fast reactors (EBR-II, ASTRID, ZPR, AFR), molten salt reactors (ThorCon), micro reactors, etc. as well as various benchmark problems for LWRs, MSRs, and SFRs.

A connection to the `MOOSE` framework is under development via the `Warthog` application which is a interfacing code for coupling `PROTEUS` and `BISON`. Progress will be made on a `MOOSE` interface tool for `PROTEUS` in FY19. In addition, an option for generating `PROTEUS` inputs is being developed in the NEAMS Workbench. `PROTEUS-SN` is connected to the thermal hydraulics code `Nek5000` and structural mechanics code `Diablo` through a MOAB interface.

Table 5.2: Different driver codes compared to the relevant success metrics. ●= Readily available or otherwise best case scenario, ◐= adequate performance or model implementation, ○= not viable.

Metric	`MCNP`	`Serpent`	`OpenMC`	`RATTLESNAKE/ MAMMOTH`	`PROTEUS`
Unstructured mesh	●	●	○	●	●
Nodal displacements	◐	○	○	●	●
Temperature dependency	●	●	●	●	●
Steady State	●	●	●	●	●
Transient	○	◐	●	●	●
Elemental state variables	◐	?	◐	●	●
Thermal scattering cross sections, e.g. $S(\alpha, \beta)$	●	●	●	N/A	●
Code Maturity	●	●	◐	◐	◐
Code Flexibility	◐	◐	●	●	◐
Coupling Interface	◐	◐	●	●	○
Ease of use	◐	●	●	●	?
Source code	●	●	●	●	●
Cost	●	●	●	●	●
Developer interaction	●	○	◐	●	●
Massively Parallelizable	◐	●	●	●	●

5.3 Heat pipe codes

5.3.1 SOCKEYE

SOCKEYE is a joint LANL and INL Heat pipe analysis program built on top of the MOOSE framework [26]. As a MOOSE-based application, SOCKEYE readily couples to MOOSE for thermal mechanics, and the greater simulation framework of BISON, Rattlesnake and Mammoth. SOCKEYE is a derivative of RELAP-7 using the pipe component of RELAP-7 to develop concentric annular cylinders to approximate heat pipe geometry. Thus, SOCKEYE is identical in structure to RELAP-7 and will provide cohesive coupling with RELAP-7. SOCKEYE has been prototyped and demonstrated and benchmarked against a LANL code employing simplified models. SOCKEYE has also been tightly coupled to the BISON nuclear fuels performance application. A proof of concept has been demonstrated with hexagonal shaped metal fuel. Further plans include coupling with RELAP-7 to provide a super critical CO_2 Brayton power generation loop. The SOCKEYE application is being developed under NEAMS and with a GAIN voucher. Efforts requiring SOCKEYE include LANL/INL's micro-reactor, MegaPower, ARPA-E MEITNER Westinghouse award, and Oklo, Inc.

5.3.2 HTPipe

HTPipe is a Los Alamos developed steady-state heat pipe analysis program developed starting in 1976 and carried throughout much of the 80's. HTPipe calculates pressure and temperature profiles based on user specified boundary conditions, which include source and sink temperature, or power throughput and evaporator exit temperature. Additionally it performs wicking, boiling and viscous limit calculations, and includes entrainment limit and condenser pressure recovery correlations. The code is written in FORTRAN77 with a text based input format.

5.3.3 HPApprox

HPApprox is a quasi steady-state approximation heat pipe analysis program for a fixed conductance alkali metal heat pipe. A one-dimensional, lumped capacitance solution is coupled to analytical, laminar, incompressible, viscous limit and condenser boundary heat transfer relations. Although this approximation considers mechanisms essential to heat pipe transients, it ignores most important details and is not suited to rapid transients, gas loaded heat pipes, or heat pipes with strongly coupled condensers.

5.4 Toolsets

Due to the maturity of the coupling infrastructure of the MOOSE based applications, the INL tool-set MOOSE-MCNP-RATTLESNAKE-MAMMOTH-SOCKEYE is likely the only code suite that can handle the quantitative simulation of the eVinci core within the time constrains of the MEITNER program. Benefiting from building built on top of the same framework, the interface between MOOSE-RATTLESNAKE-MAMMOTH-SOCKEYE should be relatively straightforward. The coupling between MCNP is likely the weakest link in the tool-set, necessitating Serpent as a backup code to

Table 5.3: Different heat pipe codes compared to the relevant success metrics. ●= Readily available or otherwise best case scenario, ◐= adequate performance or model implementation, ○= not viable.

Metric	SOCKEYE	HTPIPE	HTApprox
Double-ended heat pipe	◐	○	○
Analytical solution	●	●	●
Numerical solution	◐	◐	○
Code Maturity	◐	●	○
Code Flexibility	●	◐	○
Coupling Interface	●	○	○
Ease of use	◐	●	◐
Source code	●	●	●
Cost	●	●	●
Developer interaction	●	○	●
Massively Parallelizable	●	○	○
Run time	◐	●	●

generate cross-sections for the INL codes.

The `Abaqus+MCNP` toolkit will be used for independent comparison due to the familiarity of use with micro-reactors at LANL. It is not expected that the `Abaqus+MCNP` toolkit will be able to handle the complex analysis required to prove self-regulation of the eVinci core. In addition, although it is unlikely the `Proteus+MOOSE` tool-set will be able to provide coupled simulations with the limited project time, ongoing work with the toolkit will continue independently from MEITNER, may provide another independent assessment tool.

6 Assessment Problem

For Task 2, an assessment problem consisting of a unit assembly for a LANL design of a moderated micro-reactor will be used to exercise the MOOSE-based tool-set. Once success is shown with the smaller unit assembly, a full core of the LANL design can be used in place of better or protected information about the actual eVinci core.

In order to avoid proprietary information complexities, the LANL empire design from Fig. 3.2 will be utilized for an initial assessment. The design assumes a moderated neutron spectrum coupled to a temperature heat sink (i.e. simulated heat pipe). A single unit assembly defines the initial assessment problem by utilizing a reflecting boundary condition radially, and a vacuum boundary condition axially. The fuel selection will consider high assay low-enriched uranium (HALEU) uranium nitride fuel with nominal density. The monolith will be assumed to be fabricated from stainless steel with typical material properties. The unit assembly should exhibit heat pipe failure adequately, load-following capacity, and other desired attributes discussed previously. Adiabatic conditions will be assumed, with all heat creation from the fuel deposited into the unit assembly and removed through the heat pipes (i.e. no radiative losses).

The unit assembly will be tested via multiple simulation scenarios to assess the performance of tool-set. In a fixed unit assembly configuration, power is exclusively tied to the heat pipe temperature of the unit. As heat pipe power draw increases, the heat pipe will drop in temperature which in turn will cool the unit by some margin. Material contraction and temperature decreases will produce a positive reactivity feedback in the core, increasing the reactor power. This power increase then heats the unit to a subcritical state (due to expansion and potential doppler broadening) which decreases power slightly from the maxima, cooling down the unit assembly. A transient situation will result in power oscillations that dampen to a new steady-state power draw from the core matching the heat pipe power draw. This dampening oscillation toward a new steady-state power should be adequately shown by each coupling strategy to demonstrate power load following, for example, Fig. 6.1.

A heat pipe failure scenario will also be examined (i.e. boundary condition removal). The analysis will run at a steady-state temperature with instantaneous or gradual failure depending on criteria. The failure should exhibit the resulting temperature distribution, displacement, and subsequent power draw adjustment from the heat pipes. The modeling outcome should demonstrate the assembly capacity to respond to the described accident scenario.

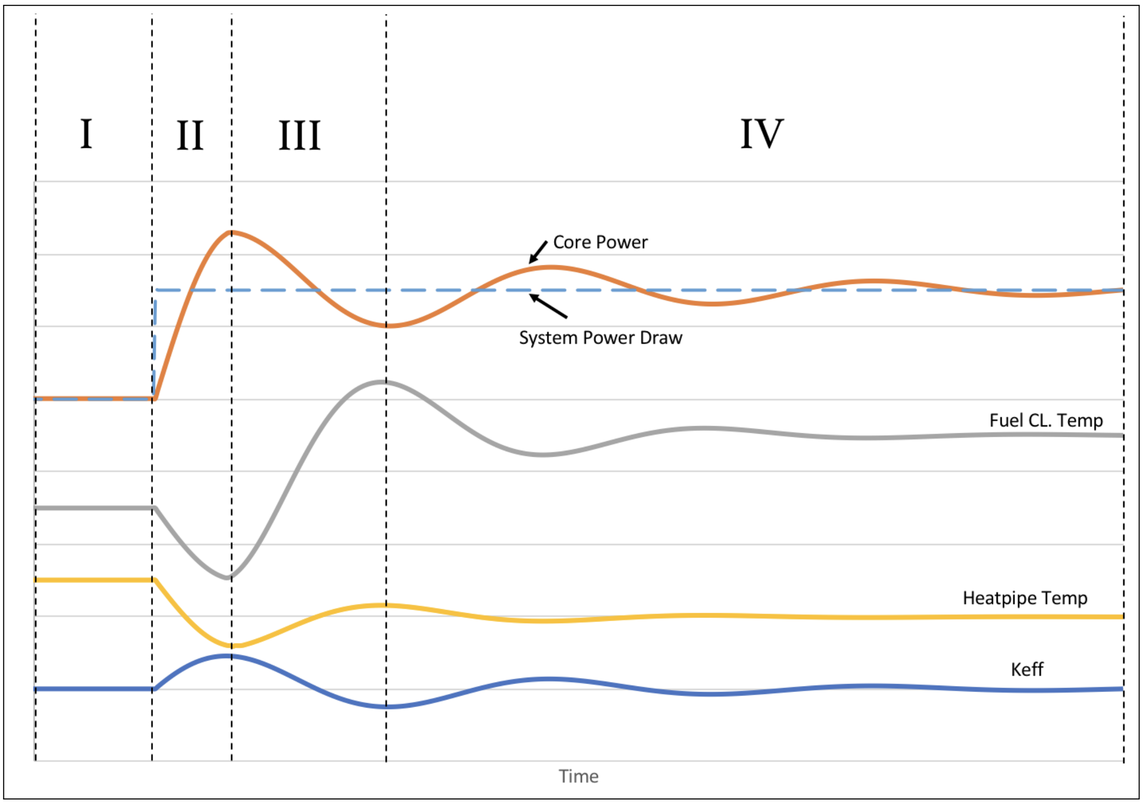


Figure 6.1: Example of a unit assembly transient.

7 Conclusions

Fundamentally, the attractiveness of heat pipe micro-reactors comes from the idea that the core is inherently self-regulating, simplifying the reactor design and requiring significantly fewer safety related components. While the WEC Design Team is focused on the experimental and fabrication tasks to ensuring self-regulation, the MEITNER Resource Team is focused on utilizing available codes to computationally show the core is indeed self-regulating. This requires the combination of fundamentally different codes to simulate the feedback mechanism between heat generation, temperature, and density.

Simulating the defining physics of self-regulation in a heat pipe cooled micro-reactor requires the coupling of three discrete simulation spaces: a master thermo-mechanical FEM code (e.g. `ANSYS`, `MOOSE`, `ABAQUS`), a temperature and spatially dependent neutronics calculation (e.g. `MCNP`, `Serpent`, `RATTLESNAKE`, `PROTEUS`, or combination of several core physics codes), and a heat pipe boundary condition definition (e.g. `SOCKEYE`, `HTPIPE`). Different toolsets can be combined between the separate regimes to leverage the physics provided by each code (e.g. `ABAQUS` + `MCNP` + `SOCKEYE`, `MOOSE` based animals).

During the exploration of codes in Task 1, it became clear that only the INL `MOOSE`-based tool-suite showed promise in producing results within the limited timeframe of the project. As a result, Task 2 will focus on the application of the INL codes to the assessment case in order to force any complications and issues with the M&S to the surface early within the project such that appropriate resources could be redirected.

The `Abaqus+MCNP` toolkit will be used for independent comparison due to the familiarity of use with micro-reactors at LANL. It is not expected that the `Abaqus+MCNP` toolkit will be able to handle the complex analysis required to prove self-regulation of the eVinci core. In addition, although it is unlikely the `Proteus+MOOSE` tool-set will be able to provide coupled simulations with the limited project time, ongoing work with the toolkit will continue independently from MEITNER, may provide another independent assessment tool.

For Task 2, an assessment problem consisting of a unit assembly for a LANL design of a moderated micro-reactor will be used to exercise the `MOOSE`-based tool-set. Once success is shown with the smaller unit assembly, a full core of the LANL design can be used in place of better or protected information about the actual eVinci core.

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